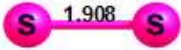
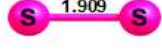
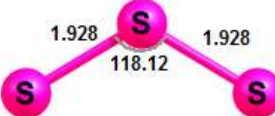
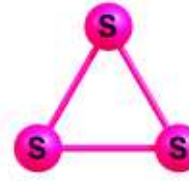


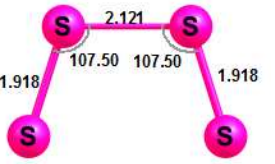
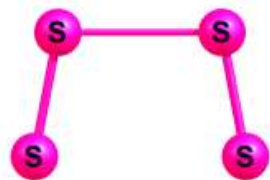
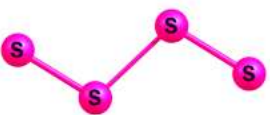
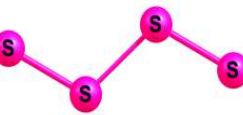
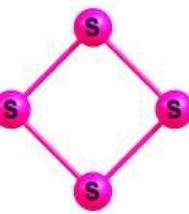
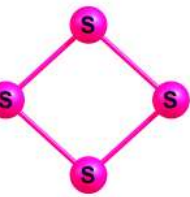
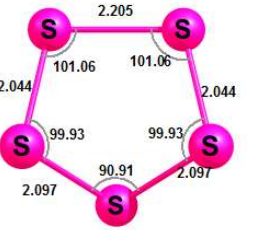
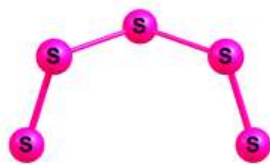
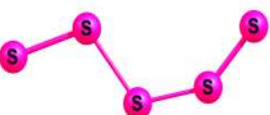
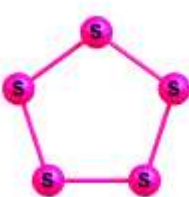
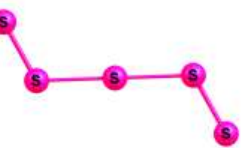
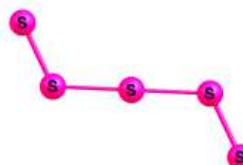
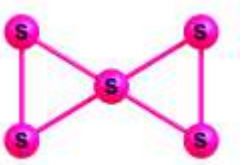
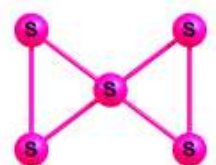


Table S1: Optimized lower/low energy isomers of S_n at the B3LYP method with the total energy (a.u) and the relative energy difference between the adjacent isomers (eV).

| | | | | | | | |
|---|--|---|---|---|--|---|---|
|  <p>$\Delta=0.000$; $D_{\infty h}$; $M=3$ $E = -798.6265042130$</p> |  <p>$\Delta=0.978$, $D_{\infty h}$; $M=1$ $E = -798.5905474904$</p> | | | | | | |
|  <p>$\Delta=0.000$; C_{2v}; $M=1$ $E = -1197.9459740390$</p> |  <p>$\Delta=0.343$; D_{3h}; $M=1$ $E = -1197.9333781446$</p> |  <p>$\Delta=0.379$; C_{2v}; $M=3$ $E = -1197.9194344297$</p> |  <p>$\Delta=0.310$; C_{2v}; $M=3$ $E = -1197.9080242152$</p> | | | | |
|  <p>$\Delta=0.000$; C_{2v}; $M=1$ $E = -1597.2731961853$</p> |  <p>$\Delta=0.186$; C_{2v}; $M=3$ $E = -1597.2663524520$</p> |  <p>$\Delta=0.070$; C_{2h}; $M=3$ $E = -1597.26379520$</p> |  <p>$\Delta=0.032$; C_{2h}; $M=1$ $E = -1597.2625993503$</p> |  <p>$\Delta=0.798$; D_{4h}; $M=1$ $E = -1597.2332537899$</p> |  <p>$\Delta=0.191$ D_{2h}; $M=3$ $E = -1597.2262423565$</p> | | |
|  <p>$\Delta=0.000$; C_s; $M=1$ $E = -1996.6120966839$</p> |  <p>$\Delta=0.636$; C_s; $M=3$ $E = -1996.5887088084$</p> |  <p>$\Delta=0.035$; C_s; $M=3$ $E = -1996.5874261138$</p> |  <p>$\Delta=0.888$; D_{5h}; $M=1$ $E = -1996.5547976417$</p> |  <p>$\Delta=0.273$; S_2; $M=3$ $E = -1996.5447584903$</p> |  <p>$\Delta=0.191$; S_2; $M=1$ $E = -1996.5377193256$</p> |  <p>$\Delta=2.607$; D_{2h}; $M=1$ $E = -1996.4419226917$</p> |  <p>$\Delta=0.748$; D_{2h}; $M=3$ $E = -1996.4144291259$</p> |

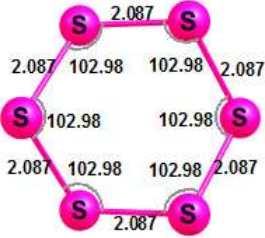
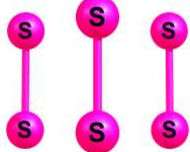
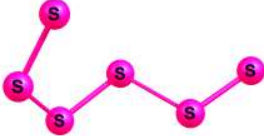
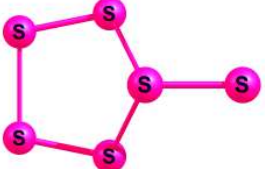
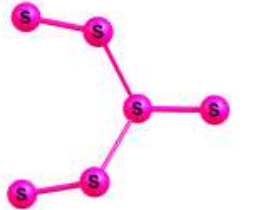

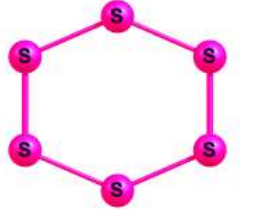
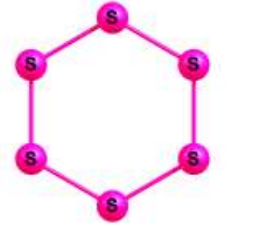
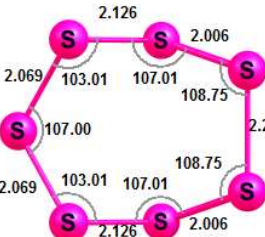
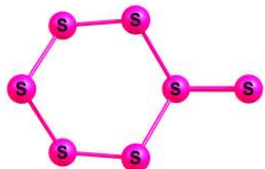
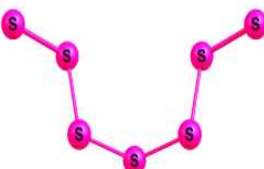
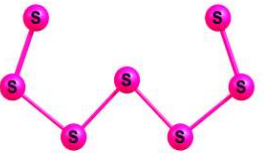
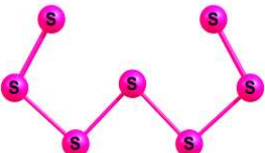
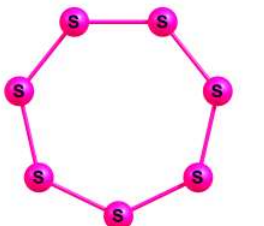

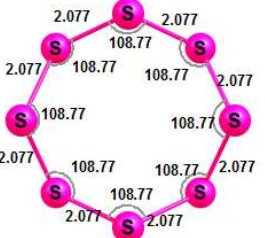
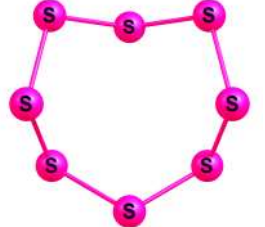
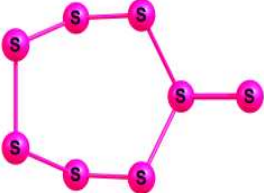
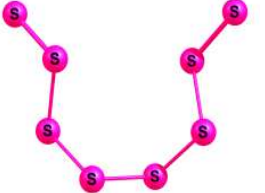

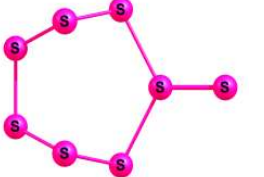
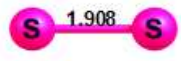
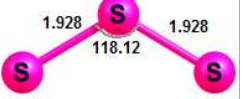
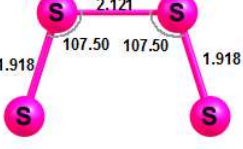
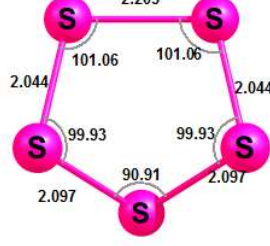
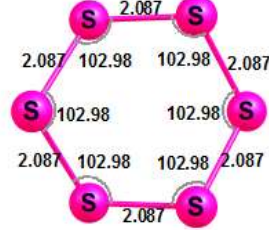
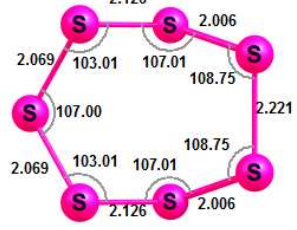
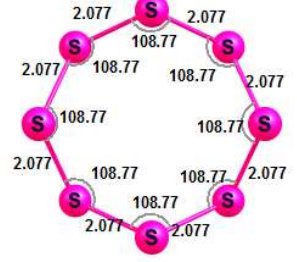
| | | | | | | | |
|---|---|---|---|---|--|--|--|
|  <p>$\Delta=0.000$; D_3; $M=1$ $E = -2395.9546151953$</p> |  <p>$\Delta=0.726$; C_s; $M=1$ $E = -2395.9279433016$</p> |  <p>$\Delta=0.231$; C_s; $M=3$ $E = -2395.9194362792$</p> |  <p>$\Delta=0.155$; C_s; $M=1$ $E = -2395.9137465697$</p> |  <p>$\Delta=0.569$; C_s; $M=3$ $E = -2395.8928318869$</p> |  <p>$\Delta=0.025$; C_2; $M=1$ $E = -2395.8919256164$</p> |  <p>$\Delta=1.005$; D_{2h}; $M=3$ $E = -2395.8550000034$</p> |  <p>$\Delta=0.517$; D_{6h}; $M=1$ $E = -2395.8360154235$</p> |
|  <p>$\Delta=0.000$; C_s; $M=1$ $E = -2795.2845812095$</p> |  <p>$\Delta=0.837$; C_s; $M=1$ $E = -2795.2538193051$</p> |  <p>$\Delta=0.256$; C_s; $M=3$ $E = -2795.2444238888$</p> |  <p>$\Delta=0.717$; C_2; $M=3$ $E = -2795.2180756938$</p> |  <p>$\Delta=0.396$; C_2; $M=1$ $E = -2795.2035345815$</p> |  <p>$\Delta=2.899$; D_{7h}; $M=1$ $E = -2795.0969897967$</p> |  <p>$\Delta=2.274$; D_{2h}; $M=1$ $E = -2795.0134044245$</p> | |
|  <p>$\Delta=0.000$; D_{4d}; $M=1$ $E = -3194.6246531083$</p> |  <p>$\Delta=0.484$; C_s; $M=1$ $E = -3194.6068623106$</p> |  <p>$\Delta=0.801$; C_s; $M=1$ $E = -3194.5774178919$</p> |  <p>$\Delta=0.128$; C_2; $M=3$ $E = -3194.5727057684$</p> |  <p>$\Delta=0.291$; C_2; $M=1$ $E = -3194.5620024964$</p> |  <p>$\Delta=0.560$; C_s; $M=3$ $E = -3194.5414145380$</p> | | |

Table S2: Vibrational Frequency of $S_{n=2-8}$ clusters at the B3LYP method.

| | | | | | | | |
|--------------------------------|---|---|--|---|---|---|---|
| $S_{n=2-8}$ |  |  |  |  |  |  |  |
| Frequency (cm^{-1}) | 716 | 260, 595, 683 | 108, 208, 330, 372, 648, 674 | 85, 231, 284, 318, 334, 417, 425, 502, 515 | <i>i</i> 23, 160, 161, 262, 271, 312, 348, 437, 444, 456, 457, 476 | 58, 125, 155, 167, 193, 233, 266, 289, 336, 367, 376, 448, 478, 516, 524 | <i>i</i> 411, <i>i</i> 406, 190, 190, 213, 241, 247, 247, 384, 399, 404, 412, 412, 464, 464, 471, 491, 494, |